Supplementary Material for Organic & Biomolecular Chemistry

Supplementary data

Imidoylketene - α-oxoketenimine and α-oxoketene-α-oxoketene rearrangements.

1,3-Shift of substituted phenyl groups

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Computational data for all species in Table 1.

Coordinates and energies (absolute energies and the sum of electronic energy and zero-point vibrational energies (ZPVE) in hartrees) of all species in Table 1 and imaginary frequencies for transition states (method B3LYP/6-31G and B3LYP/6-311+G(3df,2p)//B3LYP/6-31G** as indicated)**.

a: Diphenylimidoylketene 1 H/H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.088976	1.533528	-0.109680
2	8	0.217929	2.659716	-0.140194
3	7	0.093932	-2.031153	-0.318699
4	1	0.898042	-2.663942	-0.325578
5	6	-0.503232	0.264217	-0.071810
6	6	0.497560	-0.824154	-0.145943
7	6	-1.982194	0.054914	-0.024164
8	6	-2.536594	-0.988960	0.734031
9	6	-2.846577	0.925207	-0.707230
10	6	-3.918693	-1.149862	0.800993
11	1	-1.881276	-1.681149	1.246594
12	6	-4.229482	0.769548	-0.623161
13	1	-2.434173	1.723578	-1.318777
14	6	-4.771982	-0.271119	0.130135
15	1	-4.331079	-1.967307	1.385538
16	1	-4.879827	1.455122	-1.158592
17	1	-5.848505	-0.401200	0.188993
18	6	1.944634	-0.446343	-0.031016
19	6	2.416721	0.346416	1.026181

20	6	2.861183	-0.935735	-0.974918
21	6	3.776034	0.641739	1.135178
22	1	1.723969	0.709320	1.779421
23	6	4.216588	-0.631427	-0.869566
24	1	2.499659	-1.540356	-1.801731
25	6	4.677536	0.157475	0.186945
26	1	4.129974	1.246035	1.965048
27	1	4.912759	-1.005307	-1.614451
28	1	5.734334	0.392872	0.270126

Energy = -708.173551
E+ZPVE = -707.955193
Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -708.3928028
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -708.1744458

a: oxoketenimine 2 H/H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.491442	-0.714779	-0.277798
2	8	0.154821	-1.850770	-0.588560
3	7	0.168599	2.795289	-0.501971
4	1	0.436995	3.415217	0.264040
5	6	-0.526802	0.370912	-0.140585
6	6	-0.133344	1.641495	-0.243040
7	6	1.942778	-0.401040	-0.055013
8	6	2.887244	-1.101458	-0.820710
9	6	2.387725	0.495620	0.926695
10	6	4.248245	-0.877277	-0.637218
11	1	2.531424	-1.815980	-1.555277
12	6	3.753075	0.705151	1.122757
13	1	1.668933	1.000210	1.564477
14	6	4.684175	0.028021	0.334737
15	1	4.971584	-1.411414	-1.246096
16	1	4.089042	1.389648	1.896090
17	1	5.746745	0.196842	0.483208
18	6	-1.981971	0.069118	-0.015539
19	6	-2.423521	-1.098221	0.628460
20	6	-2.942095	0.964695	-0.514908
21	6	-3.786501	-1.352843	0.769782
22	1	-1.700417	-1.811346	1.003153
23	6	-4.303304	0.709072	-0.364998
24	1	-2.619384	1.863871	-1.032258
25	6	-4.732722	-0.452439	0.278471
26	1	-4.108712	-2.262334	1.268634
27	1	-5.028064	1.414548	-0.761099

28	1	-5.793456	-0.656290	0.390842

Energy = -708.171588
E+ZPVE = -707.954157
Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = --708.3901038
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -- 708.1726728

a: TS1 connecting diphenylimidoylketene 1 and oxoketenimine 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.367768	-1.059897	-0.000045
2	8	0.410206	-2.268927	-0.000074
3	7	0.472171	2.293878	0.000044
4	1	1.362243	2.772373	0.000133
5	6	-0.555183	-0.005206	-0.000010
6	6	0.380036	1.052920	0.000026
7	6	-2.013878	0.016355	-0.000004
8	6	-2.728556	1.228672	-0.000025
9	6	-2.735046	-1.193892	0.000024
10	6	-4.121803	1.226160	-0.000017
11	1	-2.183943	2.167485	-0.000044
12	6	-4.127274	-1.184811	0.000031
13	1	-2.191572	-2.133260	0.000036
14	6	-4.829464	0.022682	0.000011
15	1	-4.657365	2.171616	-0.000032
16	1	-4.667068	-2.127808	0.000050
17	1	-5.915500	0.025277	0.000016
18	6	1.781255	-0.128035	-0.000008
19	6	2.520091	-0.090807	-1.218852
20	6	2.520075	-0.090890	1.218848
21	6	3.902380	0.010001	-1.218126
22	1	1.974260	-0.135202	-2.157552
23	6	3.902364	0.009919	1.218146
24	1	1.974232	-0.135353	2.157538
25	6	4.593691	0.063286	0.000016
26	1	4.451059	0.044106	-2.154363
27	1	4.451032	0.043959	2.154392
28	1	5.677042	0.142334	0.000026

Energy = -708.112845
E+ZPVE = -707.898328
Imaginary frequency: - 460.3
Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -708.3311115
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -728.1165945

b: Diphenylimidoylketene 1 substituent- C_6F_5 as the non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.964770	1.409523	-0.918072
2	8	-1.323621	2.308180	-1.566039
3	7	-0.943604	-1.161758	1.551001
4	1	-1.682042	-1.687596	2.024970
5	6	-0.518983	0.378094	-0.197395
6	6	-1.451217	-0.423367	0.634549
7	6	0.948051	0.168691	-0.135475
8	6	1.505225	-1.095930	-0.366104
9	6	1.831151	1.204568	0.186967
10	6	2.872847	-1.323488	-0.251946
11	6	3.204637	1.002857	0.285012
12	6	3.725829	-0.270219	0.071790
13	6	-2.914862	-0.299399	0.350909
14	6	-3.416617	-0.381886	-0.957093
15	6	-3.814422	-0.136349	1.416153
16	6	-4.789506	-0.305793	-1.192384
17	1	-2.734396	-0.537369	-1.787260
18	6	-5.184131	-0.050841	1.177463
19	1	-3.430665	-0.055504	2.429067
20	6	-5.674928	-0.136605	-0.127530
21	1	-5.166283	-0.384313	-2.207649
22	1	-5.868569	0.088777	2.008799
23	1	-6.742885	-0.071441	-0.312535
24	9	5.041401	-0.479618	0.165268
25	9	1.356647	2.443291	0.399350
26	9	4.020609	2.018673	0.589552
27	9	3.377107	-2.542520	-0.474575
28	9	0.723036	-2.120363	-0.717944

Energy = -1204.2963598
E+ZPVE = -1204.119141

b: oxoketenimine 2 with C_6F_5 as the non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.435324	-0.346313	0.588109
2	8	-0.990853	-1.091354	1.448938
3	7	-1.299129	2.759531	-1.121871
4	1	-1.607992	2.875154	-2.087137

5	6	-0.494472	0.539278	-0.173950
6	6	-0.919229	1.667894	-0.741616
7	6	-2.903692	-0.285676	0.305855
8	6	-3.783061	-0.547507	1.367670
9	6	-3.424684	-0.045315	-0.973408
10	6	-5.158804	-0.529727	1.160964
11	1	-3.365561	-0.760209	2.345953
12	6	-4.803688	-0.045445	-1.182261
13	1	-2.753032	0.100053	-1.813365
14	6	-5.671797	-0.276946	-0.114598
15	1	-5.833220	-0.718256	1.990788
16	1	-5.199519	0.125715	-2.178858
17	1	-6.745591	-0.270257	-0.277029
18	6	0.954933	0.233519	-0.127192
19	6	1.425589	-1.051146	-0.427262
20	6	1.908548	1.187009	0.246648
21	6	2.774955	-1.378366	-0.344781
22	6	3.265676	0.885622	0.318632
23	6	3.699305	-0.404858	0.027899
24	9	4.998605	-0.706437	0.096672
25	9	4.150615	1.823721	0.675892
26	9	1.524737	2.437236	0.544945
27	9	0.569527	-2.000979	-0.822172
28	9	3.192083	-2.614678	-0.640116

Energy = -1204.293692
E+ZPVE = -1204.117491

b: TS1 with C_6F_5 as the non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.404913	-0.884105	0.611184
2	8	1.451330	-1.886005	1.278906
3	7	1.492936	1.918227	-1.254772
4	1	2.375604	2.273227	-1.595877
5	6	0.483866	-0.000483	0.026116
6	6	1.409513	0.882737	-0.576537
7	6	-0.977248	0.009772	0.007907
8	6	-1.717230	1.196971	0.108890
9	6	-1.711344	-1.180963	-0.103161
10	6	-3.108180	1.206148	0.083347
11	6	-3.102255	-1.195129	-0.102494
12	6	-3.805204	0.004411	-0.015348
13	6	2.807459	-0.102820	0.074596
14	6	3.533572	-0.755340	-0.965151
15	6	3.557903	0.607984	1.057533

16	6	4.915250	-0.674059	-1.035187
17	1	2.979302	-1.317076	-1.712410
18	6	4.938833	0.690433	0.983780
19	1	3.022221	1.096153	1.867258
20	6	5.617753	0.051966	-0.063669
21	1	5.454618	-1.170729	-1.835794
22	1	5.496781	1.241529	1.734468
23	1	6.700535	0.116603	-0.120054
24	9	-5.142196	0.001976	-0.026451
25	9	-3.779846	2.360791	0.180173
26	9	-1.082412	2.369690	0.243085
27	9	-1.068778	-2.350229	-0.224226
28	9	-3.768530	-2.351606	-0.209947

Energy = -1204.2322753
E+ZPVE = -1204.058890
Imaginary frequency: - 451.8

c: Diphenylimidoylketene 1 substituent- F on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.333319	1.565602	-0.089637
2	8	0.658060	2.687057	-0.109501
3	7	0.442881	-2.003417	-0.308205
4	1	1.231337	-2.655493	-0.314600
5	6	-0.102851	0.303420	-0.069547
6	6	0.874994	-0.805669	-0.140243
7	6	-1.584763	0.117227	-0.040835
8	6	-2.166137	-0.906140	0.726703
9	6	-2.427793	0.984217	-0.753738
10	6	-3.548842	-1.056932	0.778645
11	1	-1.529481	-1.597845	1.262479
12	6	-3.814411	0.854345	-0.694891
13	1	-1.997815	1.766688	-1.372747
14	6	-4.353414	-0.169935	0.071720
15	1	-4.008166	-1.848160	1.361113
16	1	-4.470896	1.520852	-1.243197
17	6	2.329592	-0.459072	-0.027308
18	6	2.819930	0.324506	1.028422
19	6	3.233912	-0.968609	-0.972355
20	6	4.185299	0.591774	1.134443
21	1	2.136826	0.701817	1.783400
22	6	4.595519	-0.692433	-0.869706
23	1	2.858536	-1.566416	-1.797941
24	6	5.074701	0.087960	0.185009

25	1	4.553274	1.189237	1.963121
26	1	5.282386	-1.081699	-1.615313
27	1	6.136305	0.301343	0.266014
28	9	-5.694587	-0.313824	0.126780

Energy = - 807.4052433
E+ZPVE = - 807.195143

c: oxoketenimine 2 with -F on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.863468	-0.689814	-0.280655
2	8	0.491988	-1.813890	-0.595897
3	7	0.648521	2.833619	-0.461723
4	1	0.924649	3.436074	0.315517
5	6	-0.122045	0.425772	-0.146817
6	6	0.309569	1.685932	-0.221866
7	6	2.322018	-0.421986	-0.049388
8	6	3.248138	-1.142791	-0.818626
9	6	2.789292	0.451380	0.942973
10	6	4.614415	-0.960666	-0.628030
11	1	2.874480	-1.839243	-1.561634
12	6	4.159459	0.618203	1.146074
13	1	2.083514	0.970755	1.583467
14	6	5.073072	-0.078382	0.354561
15	1	5.324001	-1.509924	-1.239580
16	1	4.512577	1.284546	1.927536
17	1	6.139565	0.057297	0.508590
18	6	-1.586382	0.163467	-0.055579
19	6	-2.075640	-0.992278	0.576494
20	6	-2.511491	1.082408	-0.578143
21	6	-3.445155	-1.219424	0.687981
22	1	-1.382643	-1.725487	0.968084
23	6	-3.883412	0.870639	-0.465672
24	1	-2.155494	1.973365	-1.087000
25	6	-4.329550	-0.282330	0.168035
26	1	-3.831192	-2.110106	1.171542
27	1	-4.601444	1.575609	-0.870034
28	9	-5.657566	-0.499765	0.277190

Energy = -807.4033482
E+ZPVE = -807.194160

c: TS1 with -F on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.767993	-1.061087	-0.000005
2	8	-0.806955	-2.270754	-0.000005
3	7	-0.866079	2.293095	-0.000004
4	1	-1.754156	2.775377	0.000012
5	6	0.155108	-0.007039	-0.000003
6	6	-0.778966	1.051397	-0.000001
7	6	1.613930	0.013381	-0.000002
8	6	2.330736	1.224545	-0.000005
9	6	2.334942	-1.197165	0.000002
10	6	3.723820	1.229700	-0.000004
11	1	1.789104	2.164724	-0.000008
12	6	3.726981	-1.198556	0.000002
13	1	1.792495	-2.136803	0.000003
14	6	4.401790	0.016848	0.000000
15	1	4.285862	2.157465	-0.000006
16	1	4.291257	-2.124954	0.000005
17	6	-2.178237	-0.129297	0.000000
18	6	-2.917301	-0.090774	1.219151
19	6	-2.917308	-0.090771	-1.219148
20	6	-4.299182	0.013313	1.218365
21	1	-2.371508	-0.136591	2.157784
22	6	-4.299188	0.013317	-1.218354
23	1	-2.371519	-0.136585	-2.157784
24	6	-4.990161	0.068259	0.000007
25	1	-4.847944	0.048607	2.154466
26	1	-4.847955	0.048614	-2.154452
27	1	-6.073315	0.149849	0.000010
28	9	5.754672	0.018693	0.000001

Energy = -807.3447238
E+ZPVE = -807.138512
Imaginary frequency: - 455.1

d: Diphenylimidoylketene 1 with substituent- CHO on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.652641	1.496222	-0.190474
2	8	0.978292	2.613166	-0.255060
3	7	0.858463	-2.061202	-0.347317
4	1	1.673740	-2.679204	-0.338778

5	6	0.218251	0.231703	-0.113574
6	6	1.235124	-0.847650	-0.165823
7	6	-1.256979	0.039978	-0.050323
8	6	-1.816943	-1.118918	0.515414
9	6	-2.124261	1.045778	-0.529096
10	6	-3.198686	-1.253999	0.600908
11	1	-1.166029	-1.911788	0.855798
12	6	-3.499452	0.909856	-0.430778
13	1	-1.713136	1.938181	-0.993890
14	6	-4.053878	-0.247240	0.136878
15	1	-3.622000	-2.155825	1.037511
16	1	-4.168358	1.681420	-0.798134
17	6	2.672905	-0.444607	-0.022601
18	6	3.110606	0.343352	1.053085
19	6	3.614323	-0.907648	-0.955291
20	6	4.462271	0.660255	1.190976
21	1	2.397667	0.684854	1.797615
22	6	4.961894	-0.581041	-0.820770
23	1	3.278762	-1.508469	-1.795671
24	6	5.388927	0.202813	0.253672
25	1	4.790620	1.260013	2.034409
26	1	5.678290	-0.933467	-1.556717
27	1	6.439690	0.455254	0.359297
28	6	-5.517993	-0.406690	0.238609
29	8	-6.333837	0.415487	-0.136892
30	1	-5.846628	-1.364750	0.700511

Energy = -821.4989657
E+ZPVE = -821.271309

d: oxoketenimine 2 with -CHO on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.217465	-0.709964	-0.321584
2	8	0.879267	-1.837065	-0.660516
3	7	0.956648	2.792044	-0.590132
4	1	1.227541	3.428968	0.160077
5	6	0.205897	0.388376	-0.205848
6	6	0.627277	1.651078	-0.320909
7	6	2.661273	-0.412909	-0.043638
8	6	3.626375	-1.121968	-0.775194
9	6	3.077456	0.477074	0.956976
10	6	4.981495	-0.912622	-0.539150
11	1	3.291561	-1.830247	-1.525462
12	6	4.436351	0.671471	1.205275
13	1	2.340517	0.986936	1.569507

14	6	5.389271	-0.014104	0.451186
15	1	5.721914	-1.452734	-1.121455
16	1	4.750050	1.350099	1.992865
17	1	6.447070	0.142992	0.640440
18	6	-1.252267	0.119547	-0.089652
19	6	-1.726795	-1.100823	0.422778
20	6	-2.190477	1.104406	-0.465213
21	6	-3.094097	-1.317925	0.558571
22	1	-1.026422	-1.878156	0.695920
23	6	-3.551053	0.885142	-0.323312
24	1	-1.842513	2.045667	-0.880709
25	6	-4.019144	-0.333177	0.192630
26	1	-3.449903	-2.265559	0.956465
27	1	-4.275541	1.639404	-0.613210
28	6	-5.467441	-0.577130	0.345906
29	8	-6.339819	0.223139	0.061437
30	1	-5.725910	-1.579087	0.756195

Energy = - 821.4970186
E+ZPVE = - 821.270321

d: TS1 with -CHO on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.131808	1.085518	-0.000007
2	8	1.205721	2.291959	0.000002
3	7	1.124447	-2.273104	-0.000014
4	1	1.996227	-2.784945	0.000033
5	6	0.174599	0.057934	-0.000012
6	6	1.079225	-1.030644	-0.000007
7	6	-1.277845	0.082686	-0.000006
8	6	-2.030878	-1.113092	-0.000002
9	6	-1.959934	1.318114	-0.000002
10	6	-3.415741	-1.071077	0.000004
11	1	-1.511364	-2.065731	-0.000005
12	6	-3.347648	1.348738	0.000003
13	1	-1.386661	2.239141	-0.000005
14	6	-4.092348	0.160067	0.000007
15	1	-4.004417	-1.983101	0.000007
16	1	-3.867226	2.304542	0.000004
17	6	2.507285	0.106762	-0.000003
18	6	3.244830	0.045183	1.220116
19	6	3.244841	0.045188	-1.220115
20	6	4.622281	-0.103104	1.218916
21	1	2.700948	0.108383	2.158835
22	6	4.622292	-0.103100	-1.218903

23	1	2.700969	0.108392	-2.158839
24	6	5.310638	-0.180134	0.000010
25	1	5.169965	-0.155977	2.154698
26	1	5.169985	-0.155970	-2.154680
27	1	6.390566	-0.296520	0.000014
28	6	-5.564740	0.208556	0.000003
29	8	-6.297168	-0.765699	0.000002
30	1	-5.990535	1.237858	-0.000002

Energy = -821.4401485
E+ZPVE = - 821.216019
Imaginary frequency: - 445.8

e: Diphenylimidoylketene 1 with substituent- CN on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.614046	1.536603	-0.189109
2	8	0.964841	2.646487	-0.245445
3	7	0.713067	-2.027289	-0.344918
4	1	1.505049	-2.674679	-0.330110
5	6	0.148458	0.283308	-0.122278
6	6	1.131299	-0.827549	-0.164393
7	6	-1.331740	0.127353	-0.081535
8	6	-1.928911	-0.996634	0.516540
9	6	-2.168025	1.127239	-0.612721
10	6	-3.311830	-1.108690	0.585699
11	1	-1.302995	-1.790162	0.899860
12	6	-3.550213	1.026153	-0.535467
13	1	-1.734372	1.993753	-1.104094
14	6	-4.137768	-0.098186	0.066384
15	1	-3.761034	-1.981738	1.046972
16	1	-4.179399	1.806402	-0.949835
17	6	2.579875	-0.470779	-0.013068
18	6	3.035036	0.312391	1.058864
19	6	3.512350	-0.972269	-0.934823
20	6	4.395190	0.587200	1.203619
21	1	2.328823	0.682284	1.796216
22	6	4.868704	-0.687881	-0.793290
23	1	3.163716	-1.569402	-1.772511
24	6	5.313157	0.091752	0.277157
25	1	4.736734	1.183467	2.044250
26	1	5.578533	-1.069969	-1.520714
27	1	6.370717	0.311191	0.388265
28	6	-5.563538	-0.215260	0.143170

29	7	-6.721787	-0.308648	0.207311

Energy = -800.4161739
E+ZPVE = - 800.199237

e: oxoketenimine 2 with -CN on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.115413	-0.691153	-0.322046
2	8	0.740720	-1.804530	-0.667708
3	7	0.955246	2.823671	-0.550203
4	1	1.238336	3.444090	0.209266
5	6	0.137213	0.436801	-0.203346
6	6	0.591954	1.689220	-0.297678
7	6	2.566367	-0.440657	-0.039344
8	6	3.510754	-1.173686	-0.774371
9	6	3.007260	0.429379	0.968303
10	6	4.871116	-1.006894	-0.534662
11	1	3.156207	-1.866270	-1.530191
12	6	4.370900	0.580743	1.220148
13	1	2.285236	0.956724	1.583831
14	6	5.303949	-0.128021	0.462638
15	1	5.595939	-1.565117	-1.119442
16	1	4.703603	1.243797	2.013146
17	1	6.365640	-0.004365	0.654737
18	6	-1.328762	0.204824	-0.108797
19	6	-1.842653	-0.997041	0.410078
20	6	-2.236917	1.201384	-0.511944
21	6	-3.213536	-1.189431	0.529332
22	1	-1.166761	-1.787762	0.705465
23	6	-3.607159	1.017739	-0.391125
24	1	-1.865473	2.130165	-0.934185
25	6	-4.110434	-0.184101	0.133785
26	1	-3.597002	-2.120590	0.932476
27	1	-4.293542	1.795282	-0.708659
28	6	-5.523821	-0.381005	0.261327
29	7	-6.672077	-0.537716	0.367550

Energy = -800.4142334
E+ZPVE = -800.198256

e: TS1 with -CN on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.024598	-1.065944	-0.000017
2	8	1.058052	-2.274363	-0.000036
3	7	1.116206	2.292320	0.000037
4	1	2.001665	2.780175	0.000047
5	6	0.099822	-0.009099	0.000000
6	6	1.036297	1.051451	0.000017
7	6	-1.352839	0.011068	-0.000001
8	6	-2.070050	1.224571	0.000017
9	6	-2.074256	-1.201744	-0.000019
10	6	-3.457798	1.226980	0.000016
11	1	-1.527293	2.163809	0.000031
12	6	-3.461084	-1.200375	-0.000020
13	1	-1.530860	-2.140566	-0.000033
14	6	-4.169780	0.014701	-0.000002
15	1	-4.001702	2.165793	0.000030
16	1	-4.007376	-2.137775	-0.000034
17	6	2.427149	-0.131485	-0.000001
18	6	3.166344	-0.091501	-1.220412
19	6	3.166342	-0.091541	1.220412
20	6	4.547323	0.017369	-1.219110
21	1	2.620904	-0.139602	-2.159110
22	6	4.547321	0.017329	1.219116
23	1	2.620901	-0.139672	2.159109
24	6	5.237400	0.074640	0.000004
25	1	5.096489	0.054225	-2.154753
26	1	5.096486	0.054155	2.154761
27	1	6.320227	0.159821	0.000007
28	6	-5.601391	0.017542	-0.000003
29	7	-6.765669	0.020648	-0.000003

Energy = -800.3577375
E+ZPVE = -800.144280
Imaginary frequency: -441.6

f: Diphenylimidoylketene 1 with substituent- NO_2 on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.038490	1.535968	-0.163938
2	8	1.402011	2.642156	-0.184516
3	7	1.130931	-2.016564	-0.451019

4	1	1.924464	-2.662140	-0.452266
5	6	0.558828	0.285141	-0.137929
6	6	1.542549	-0.824630	-0.214346
7	6	-0.921393	0.142705	-0.101714
8	6	-1.530288	-1.035959	0.368878
9	6	-1.747655	1.210034	-0.509331
10	6	-2.914883	-1.137366	0.437659
11	1	-0.912246	-1.875952	0.651626
12	6	-3.130235	1.120705	-0.434784
13	1	-1.306552	2.122053	-0.901362
14	6	-3.701364	-0.058352	0.040414
15	1	-3.393569	-2.039265	0.797819
16	1	-3.769652	1.936657	-0.746395
17	6	2.988389	-0.471739	-0.029123
18	6	3.427418	0.259935	1.085192
19	6	3.933581	-0.925892	-0.962372
20	6	4.784698	0.531029	1.260139
21	1	2.710664	0.592006	1.830353
22	6	5.287100	-0.644820	-0.790189
23	1	3.597308	-1.482916	-1.832091
24	6	5.715517	0.083443	0.322203
25	1	5.113942	1.086891	2.132720
26	1	6.007226	-0.989316	-1.526174
27	1	6.770872	0.300208	0.456884
28	8	-5.826679	0.810503	-0.237555
29	8	-5.639375	-1.220458	0.534543
30	7	-5.161592	-0.164442	0.117385

Energy = -912.6748117
E+ZPVE = -912.453835

f: oxoketenimine 2 with –NO_2 on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.520410	-0.667149	-0.365560
2	8	1.140243	-1.760081	-0.765504
3	7	1.395118	2.853872	-0.456109
4	1	1.678834	3.444816	0.325999
5	6	0.550406	0.464164	-0.208015
6	6	1.019250	1.714759	-0.251335
7	6	2.969513	-0.441610	-0.055443
8	6	3.916539	-1.150837	-0.810236
9	6	3.405217	0.381191	0.993416
10	6	5.275205	-1.005981	-0.547955
11	1	3.565458	-1.807369	-1.599112
12	6	4.766929	0.509983	1.267111

13	1	2.680230	0.887928	1.622711
14	6	5.703101	-0.173995	0.490805
15	1	6.002447	-1.544907	-1.147597
16	1	5.095610	1.135749	2.091444
17	1	6.763376	-0.067678	0.700243
18	6	-0.917603	0.245527	-0.130138
19	6	-1.447462	-0.981656	0.311128
20	6	-1.811262	1.280001	-0.470703
21	6	-2.821330	-1.164159	0.417372
22	1	-0.782169	-1.797948	0.555639
23	6	-3.184472	1.109389	-0.364125
24	1	-1.426269	2.228133	-0.832886
25	6	-3.675643	-0.116289	0.082058
26	1	-3.239368	-2.102868	0.758200
27	1	-3.877364	1.898732	-0.626236
28	8	-5.853097	0.643831	-0.098263
29	8	-5.532135	-1.400478	0.589211
30	7	-5.125641	-0.305415	0.198646

Energy = -912.6727817
E+ZPVE = -912.452777

f: TS1 with –NO_2 on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.438345	-1.067602	0.000007
2	8	-1.471076	-2.275589	0.000014
3	7	-1.526837	2.291610	0.000009
4	1	-2.411333	2.781413	0.000006
5	6	-0.512220	-0.010470	-0.000004
6	6	-1.449184	1.051023	0.000004
7	6	0.938608	0.009033	-0.000005
8	6	1.655421	1.224655	-0.000003
9	6	1.658856	-1.206351	-0.000008
10	6	3.043086	1.228385	-0.000004
11	1	1.112083	2.163336	-0.000001
12	6	3.045656	-1.207179	-0.000008
13	1	1.114285	-2.144298	-0.000009
14	6	3.726471	0.011749	-0.000005
15	1	3.607317	2.152458	-0.000002
16	1	3.611499	-2.130272	-0.000009
17	6	-2.838376	-0.131902	0.000006
18	6	-3.577588	-0.091290	1.220756
19	6	-3.577583	-0.091288	-1.220747
20	6	-4.958296	0.019224	1.219307
21	1	-3.032261	-0.140119	2.159475

22	6	-4.958291	0.019226	-1.219304
23	1	-3.032252	-0.140113	-2.159464
24	6	-5.648129	0.077287	0.000000
25	1	-5.507545	0.056662	2.154838
26	1	-5.507536	0.056665	-2.154838
27	1	-6.730851	0.163646	-0.000002
28	8	5.764079	1.105253	-0.000005
29	8	5.767314	-1.075361	-0.000005
30	7	5.188772	0.013990	-0.000005

Energy = -912.6168803
E+ZPVE = -912.399321
Imaginary frequency: - 437.7

g: Diphenylimidoylketene 1 with substituent - OH on migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.456658	1.508185	-0.193607
2	8	-0.127228	2.627009	-0.259471
3	7	-0.341900	-2.054644	-0.375783
4	1	0.447880	-2.705324	-0.379593
5	6	-0.894401	0.249042	-0.113677
6	6	0.088174	-0.857715	-0.194028
7	6	-2.374274	0.066592	-0.021876
8	6	-2.924238	-0.966496	0.754243
9	6	-3.244003	0.951696	-0.678820
10	6	-4.306227	-1.101753	0.865084
11	1	-2.266094	-1.670907	1.246218
12	6	-4.626191	0.821538	-0.551274
13	1	-2.836927	1.741869	-1.304473
14	6	-5.164098	-0.208080	0.220275
15	1	-4.714857	-1.911219	1.463268
16	1	-5.280178	1.518359	-1.067464
17	1	-6.240460	-0.318362	0.312921
18	6	1.538563	-0.505098	-0.077895
19	6	2.025744	0.312211	0.952110
20	6	2.461669	-1.044039	-0.991385
21	6	3.387304	0.584571	1.068701
22	1	1.341352	0.718833	1.690246
23	6	3.819070	-0.771132	-0.891452
24	1	2.100495	-1.669205	-1.802864
25	6	4.288730	0.047132	0.144269
26	1	3.748777	1.208990	1.882690
27	1	4.529724	-1.173022	-1.605590
28	8	5.630216	0.280462	0.197832
29	1	5.824706	0.862802	0.944229

Energy = -783.3945971
E+ZPVE = -783.172052

g: oxoketenimine 2 with –OH on migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.090761	-0.712403	-0.365437
2	8	-0.260186	-1.834685	-0.712701
3	7	-0.237365	2.793072	-0.616759
4	1	0.060926	3.420671	0.132160
5	6	-0.924127	0.376177	-0.193771
6	6	-0.534254	1.643927	-0.328179
7	6	1.538019	-0.416593	-0.135765
8	6	2.480911	-1.166531	-0.855809
9	6	2.003202	0.510721	0.810865
10	6	3.842647	-0.967811	-0.672898
11	1	2.121482	-1.905856	-1.563405
12	6	3.363805	0.706270	1.016195
13	1	1.295000	1.057826	1.424389
14	6	4.290021	-0.026302	0.264834
15	1	4.562884	-1.543116	-1.250726
16	1	3.728928	1.408099	1.758206
17	6	-2.372145	0.073452	-0.008482
18	6	-2.785901	-1.106846	0.630567
19	6	-3.353744	0.979992	-0.442555
20	6	-4.141110	-1.363267	0.830865
21	1	-2.047655	-1.829174	0.954856
22	6	-4.706765	0.722394	-0.234033
23	1	-3.054848	1.889985	-0.955281
24	6	-5.108026	-0.452019	0.404279
25	1	-4.440819	-2.283054	1.324923
26	1	-5.447864	1.436996	-0.580540
27	1	-6.162674	-0.657165	0.562333
28	8	5.610667	0.210949	0.494954
29	1	6.142580	-0.363792	-0.071677

Energy = - 783.3936268
E+ZPVE = -783.171977

g: TS1 with -OH on migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-0.022736	-1.095053	0.005706
2	8	-0.026851	-2.310006	0.007305
3	7	0.134010	2.264275	0.014606
4	1	1.041249	2.711171	0.028644
5	6	-0.931019	-0.021218	0.002419
6	6	0.023093	1.021275	0.009810
7	6	-2.388204	0.029049	-0.001664
8	6	-3.081964	1.253776	-0.004033
9	6	-3.131117	-1.168453	-0.003640
10	6	-4.475063	1.275771	-0.008252
11	1	-2.520359	2.182610	-0.002170
12	6	-4.522972	-1.134750	-0.008037
13	1	-2.602397	-2.116137	-0.001560
14	6	-5.204065	0.084931	-0.010373
15	1	-4.994121	2.230531	-0.009829
16	1	-5.079507	-2.068115	-0.009464
17	1	-6.289972	0.106722	-0.013666
18	6	1.370990	-0.204343	0.008761
19	6	2.118646	-0.159458	-1.209753
20	6	2.126897	-0.162841	1.225299
21	6	3.490633	-0.022600	-1.218982
22	1	1.577050	-0.218675	-2.149875
23	6	3.496862	-0.025218	1.231557
24	1	1.588349	-0.225809	2.166925
25	6	4.186914	0.047097	0.004655
26	1	4.040568	0.023546	-2.156344
27	1	4.068113	0.020359	2.152422
28	8	5.525841	0.183585	0.065097
29	1	5.899663	0.207450	-0.827378

Energy = -783.3402036
E+ZPVE = -783.120901
Imaginary frequency: -386.0

h: Diphenylimidoylketene 1 with substituent – NMe_2 on migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.183457	1.422636	-0.476119
2	8	-0.834352	2.508246	-0.731005
3	7	-1.144339	-2.124463	-0.125615
4	1	-0.367126	-2.784870	-0.040603
5	6	-1.646661	0.204654	-0.184136
6	6	-0.685038	-0.923506	-0.114715
7	6	-3.126005	0.076198	-0.026821
8	6	-3.675851	-0.834711	0.890079
9	6	-3.996518	0.894840	-0.764820

10	6	-5.056336	-0.915050	1.058913
11	1	-3.019110	-1.490602	1.446456
12	6	-5.376323	0.821318	-0.580474
13	1	-3.592053	1.587877	-1.498074
14	6	-5.913565	-0.086327	0.331949
15	1	-5.464267	-1.630309	1.767581
16	1	-6.029861	1.465472	-1.161714
17	1	-6.988658	-0.153168	0.470283
18	6	0.769073	-0.586107	-0.062445
19	6	1.288984	0.381361	0.811228
20	6	1.683531	-1.287576	-0.864018
21	6	2.651544	0.643818	0.881575
22	1	0.621484	0.918848	1.478387
23	6	3.045619	-1.029606	-0.816010
24	1	1.313451	-2.038625	-1.556689
25	6	3.570991	-0.045329	0.056518
26	1	2.999599	1.383855	1.590980
27	1	3.703496	-1.590719	-1.467580
28	7	4.925079	0.232796	0.094693
29	6	5.444259	1.158947	1.086488
30	1	5.286967	0.809352	2.118010
31	1	6.516207	1.286060	0.931114
32	1	4.976659	2.145656	0.989005
33	6	5.856394	-0.606164	-0.640546
34	1	5.646550	-0.586978	-1.716719
35	1	6.868821	-0.227468	-0.496474
36	1	5.833632	-1.655049	-0.309343

Energy = -842.1491503
E+ZPVE = - 841.857820

h: oxoketenimine 2 with –NMe_2 on migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.677895	-0.771956	-0.386991
2	8	-1.056118	-1.915660	-0.622499
3	7	-1.008624	2.681783	-1.049363
4	1	-0.668728	3.386046	-0.391323
5	6	-1.682315	0.342400	-0.296194
6	6	-1.295086	1.578151	-0.606855
7	6	0.769412	-0.473410	-0.214523
8	6	1.701200	-1.332743	-0.821647
9	6	1.270853	0.566029	0.583338
10	6	3.064520	-1.139915	-0.685145
11	1	1.325122	-2.161956	-1.411733
12	6	2.635105	0.764160	0.747219

13	1	0.585007	1.208297	1.126735
14	6	3.574765	-0.073418	0.098992
15	1	3.740605	-1.822408	-1.184673
16	1	2.970498	1.563694	1.395631
17	6	-3.118367	0.077941	0.001545
18	6	-3.502819	-1.032537	0.771157
19	6	-4.118383	0.953155	-0.455222
20	6	-4.845295	-1.250935	1.075436
21	1	-2.751973	-1.732409	1.114922
22	6	-5.458155	0.734145	-0.143272
23	1	-3.844329	1.807948	-1.067246
24	6	-5.829567	-0.370458	0.624719
25	1	-5.121358	-2.117269	1.669905
26	1	-6.213233	1.423623	-0.510187
27	1	-6.874299	-0.545942	0.863908
28	7	4.932787	0.134057	0.229009
29	6	5.427419	1.166531	1.123990
30	1	5.153001	0.982401	2.173119
31	1	6.515294	1.204673	1.060423
32	1	5.043468	2.154321	0.842197
33	6	5.871603	-0.823446	-0.333323
34	1	5.745867	-0.914889	-1.418729
35	1	6.889041	-0.478664	-0.146522
36	1	5.763841	-1.825231	0.106704

Energy = -842.1485242
E+ZPVE = -841.858006

h: TS1 with –NMe_2 on migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.794028	-1.171283	-0.000056
2	8	-0.882422	-2.388915	-0.000076
3	7	-0.485772	2.184722	-0.000024
4	1	0.454002	2.562038	0.000040
5	6	-1.658406	-0.054338	-0.000031
6	6	-0.660682	0.946212	-0.000021
7	6	-3.110813	0.063846	-0.000006
8	6	-3.750982	1.317877	0.000009
9	6	-3.906625	-1.099862	0.000006
10	6	-5.141786	1.401226	0.000038
11	1	-3.148241	2.220740	-0.000002
12	6	-5.295632	-1.004756	0.000034
13	1	-3.417310	-2.068432	-0.000007
14	6	-5.923008	0.243687	0.000051
15	1	-5.618507	2.378054	0.000050

16	1	-5.892952	-1.912834	0.000044
17	1	-7.007055	0.313299	0.000073
18	6	0.606069	-0.366378	-0.000036
19	6	1.371281	-0.322626	-1.212659
20	6	1.371254	-0.322655	1.212605
21	6	2.731222	-0.140675	-1.224289
22	1	0.838485	-0.407325	-2.156203
23	6	2.731195	-0.140709	1.224266
24	1	0.838436	-0.407368	2.156136
25	6	3.460427	-0.033794	-0.000003
26	1	3.251717	-0.091738	-2.172140
27	1	3.251676	-0.091786	2.172126
28	7	4.808112	0.158516	0.000029
29	6	5.547374	0.232320	1.257813
30	1	5.472542	-0.702214	1.826263
31	1	6.599107	0.416069	1.042253
32	1	5.181700	1.051296	1.887058
33	6	5.547439	0.232446	-1.257706
34	1	5.181735	1.051417	-1.886936
35	1	6.599145	0.416276	-1.042071
36	1	5.472727	-0.702069	-1.826203

Energy = -842.1015888
E+ZPVE = -841.813022
Imaginary frequency: -319.2355

i: Diphenylimidoylketene 1 with substituents –OH on migrating –CN on non-migrating phenyl groups

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.235480	1.498182	-0.312890
2	8	0.602204	2.600100	-0.414531
3	7	0.296465	-2.060146	-0.417271
4	1	1.080595	-2.716734	-0.391477
5	6	-0.247600	0.255434	-0.193992
6	6	0.727138	-0.865230	-0.230457
7	6	-1.727257	0.119469	-0.110684
8	6	-2.323072	-1.008301	0.481874
9	6	-2.565773	1.142218	-0.593988
10	6	-3.704685	-1.101251	0.593618
11	1	-1.697462	-1.819673	0.826207
12	6	-3.945892	1.059289	-0.475221
13	1	-2.136135	2.013702	-1.080168
14	6	-4.531651	-0.068526	0.122299
15	1	-4.151869	-1.977574	1.050688

16	1	-4.575761	1.857247	-0.853291
17	6	2.174131	-0.518415	-0.071455
18	6	2.631929	0.297936	0.973210
19	6	3.122339	-1.064825	-0.954723
20	6	3.990137	0.563229	1.132698
21	1	1.926790	0.707931	1.689848
22	6	4.476736	-0.798526	-0.811734
23	1	2.784072	-1.689467	-1.776394
24	6	4.917589	0.019220	0.237699
25	1	4.328916	1.186354	1.957131
26	1	5.207908	-1.204800	-1.502137
27	8	6.256452	0.244733	0.332242
28	1	6.434182	0.825572	1.084087
29	6	-5.955730	-0.166051	0.242792
30	7	-7.112666	-0.243329	0.342919

Energy = -875.6374326
E+ZPVE = - 875.416297

i: oxoketenimine 2 with –OH on migrating and –CN on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.719687	-0.666840	-0.446424
2	8	0.341549	-1.763894	-0.841731
3	7	0.529714	2.844405	-0.678234
4	1	0.835487	3.467672	0.070435
5	6	-0.264283	0.456039	-0.288302
6	6	0.179912	1.709320	-0.405382
7	6	2.161665	-0.427860	-0.146039
8	6	3.110134	-1.200455	-0.835090
9	6	2.614099	0.468093	0.837103
10	6	4.467475	-1.053413	-0.586150
11	1	2.758980	-1.914611	-1.572024
12	6	3.969124	0.611430	1.107910
13	1	1.898266	1.029575	1.428586
14	6	4.903331	-0.142806	0.387479
15	1	5.193134	-1.644936	-1.140002
16	1	4.323898	1.287317	1.878353
17	6	-1.723157	0.212685	-0.139298
18	6	-2.209717	-1.011715	0.353021
19	6	-2.652878	1.219506	-0.460508
20	6	-3.573108	-1.216198	0.525682
21	1	-1.518535	-1.810540	0.584452
22	6	-4.015520	1.023454	-0.286777
23	1	-2.304668	2.167164	-0.859977

24	6	-4.490898	-0.201129	0.211248
25	1	-3.934417	-2.165073	0.907449
26	1	-4.718054	1.809559	-0.541786
27	8	6.217359	0.043778	0.682892
28	1	6.757444	-0.542226	0.135663
29	6	-5.896330	-0.410868	0.393039
30	7	-7.038286	-0.578466	0.542588

Energy = - 875.6365635
E+ZPVE = -875.416341

i: TS1 with –OH on migrating and –CN on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.632962	-1.111480	0.009059
2	8	0.622519	-2.325654	0.010771
3	7	0.767680	2.253038	0.017707
4	1	1.669523	2.711736	0.025253
5	6	-0.280644	-0.038017	0.006143
6	6	0.671061	1.010081	0.011787
7	6	-1.731574	0.006384	0.002728
8	6	-2.431843	1.230229	0.001635
9	6	-2.470962	-1.196217	-0.000154
10	6	-3.819262	1.252569	-0.002625
11	1	-1.875034	2.161294	0.004373
12	6	-3.857468	-1.174733	-0.004446
13	1	-1.939005	-2.141526	0.001155
14	6	-4.548986	0.050550	-0.005905
15	1	-4.349880	2.199053	-0.003430
16	1	-4.417482	-2.104104	-0.006666
17	6	2.013520	-0.216300	0.009601
18	6	2.759250	-0.164578	-1.211959
19	6	2.771830	-0.166917	1.226484
20	6	4.127980	-0.008304	-1.223437
21	1	2.217012	-0.232906	-2.151064
22	6	4.138506	-0.009772	1.229658
23	1	2.236126	-0.238223	2.169091
24	6	4.825241	0.071966	0.000223
25	1	4.675883	0.044320	-2.161425
26	1	4.711486	0.043438	2.148926
27	8	6.159467	0.227197	0.059406
28	1	6.535943	0.256377	-0.832121
29	6	-5.980162	0.074137	-0.010903
30	7	-7.144416	0.094192	-0.015253

Energy = -875.5859048
E+ZPVE = -875.367696
Imaginary frequency: - 363.5

j: Diphenylimidoylketene 1 with substituents – NMe_2 on migrating and –CHO on non-migrating phenyl groups

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.451640	-1.036824	1.028756
2	8	-0.088436	-1.977957	1.612873
3	7	-0.336485	2.280696	-0.211142
4	1	0.461377	2.856747	-0.490337
5	6	-0.931205	0.030438	0.376377
6	6	0.061027	1.079363	0.016764
7	6	-2.404096	0.065064	0.163008
8	6	-3.094611	1.273334	-0.040408
9	6	-3.139738	-1.142307	0.164838
10	6	-4.472966	1.260839	-0.235068
11	1	-2.533537	2.197888	-0.051772
12	6	-4.512464	-1.144042	-0.013393
13	1	-2.623601	-2.090218	0.294750
14	6	-5.197998	0.063824	-0.219212
15	1	-4.997584	2.200418	-0.395092
16	1	-5.078545	-2.069990	-0.011896
17	6	1.493121	0.658781	-0.029334
18	6	1.916791	-0.510432	-0.681965
19	6	2.484727	1.474894	0.539813
20	6	3.259376	-0.854890	-0.761540
21	1	1.186021	-1.149293	-1.169063
22	6	3.828735	1.139724	0.481578
23	1	2.190108	2.381416	1.061538
24	6	4.257172	-0.044035	-0.169485
25	1	3.532350	-1.755534	-1.296416
26	1	4.549434	1.795295	0.953674
27	7	5.591043	-0.392447	-0.219862
28	6	6.005622	-1.578586	-0.950168
29	1	5.780613	-1.510440	-2.024376
30	1	7.082165	-1.710047	-0.838419
31	1	5.517627	-2.479562	-0.558674
32	6	6.600171	0.514952	0.300435
33	1	6.457228	0.705114	1.371607
34	1	7.585310	0.065794	0.172751
35	1	6.598253	1.483749	-0.219157
36	6	-6.659122	0.073204	-0.420946
37	8	-7.367826	-0.917590	-0.426297
38	1	-7.096443	1.085498	-0.574998

Energy = -955.4759574
E+ZPVE = -955.175132

j: oxoketenimine 2 with –NMe2 on migrating and –CHO on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.053304	-0.796428	-0.535533
2	8	-0.307363	-1.938641	-0.803660
3	7	-0.225088	2.607470	-1.344357
4	1	0.116835	3.345317	-0.726381
5	6	-0.958936	0.319653	-0.497053
6	6	-0.546897	1.536365	-0.856349
7	6	1.482949	-0.491175	-0.274554
8	6	2.454973	-1.356628	-0.807221
9	6	1.928578	0.564949	0.536011
10	6	3.805304	-1.155408	-0.586873
11	1	2.120391	-2.195360	-1.408625
12	6	3.278096	0.772571	0.782565
13	1	1.207103	1.213202	1.023475
14	6	4.260410	-0.073590	0.211473
15	1	4.515305	-1.840804	-1.032112
16	1	3.569212	1.584657	1.436571
17	6	-2.396379	0.090013	-0.202050
18	6	-2.839742	-1.109554	0.384105
19	6	-3.350087	1.095265	-0.476002
20	6	-4.185616	-1.285533	0.688365
21	1	-2.132678	-1.904044	0.578578
22	6	-4.688247	0.915655	-0.169442
23	1	-3.031878	2.023375	-0.941812
24	6	-5.123668	-0.281717	0.420425
25	1	-4.514678	-2.217964	1.141664
26	1	-5.421716	1.686902	-0.381974
27	7	5.604083	0.139021	0.427577
28	6	6.041194	1.217996	1.298029
29	1	5.701344	1.083593	2.334936
30	1	7.130706	1.256214	1.302145
31	1	5.674743	2.189477	0.944501
32	6	6.583830	-0.808781	-0.080032
33	1	6.539693	-0.886316	-1.173381
34	1	7.583848	-0.467949	0.188712
35	1	6.443222	-1.815080	0.338081
36	6	-6.546911	-0.483587	0.751219
37	8	-7.428772	0.335123	0.561652
38	1	-6.778259	-1.472906	1.206653

Energy = -955.4747563
E+ZPVE = -955.174975

j: TS1 with –NMe_2 on migrating and –CHO on non-migrating phenyl group

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Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.040450	1.268828	-0.000061
2	8	-0.102502	2.487275	0.000077
3	7	0.162542	-2.099362	-0.000674
4	1	1.088445	-2.510329	-0.000467
5	6	-0.940084	0.174869	-0.000191
6	6	0.028618	-0.857855	-0.000352
7	6	-2.387937	0.101258	-0.000111
8	6	-3.066689	-1.139671	-0.000262
9	6	-3.147800	1.292288	0.000132
10	6	-4.450872	-1.184314	-0.000150
11	1	-2.487557	-2.057560	-0.000465
12	6	-4.534015	1.235650	0.000218
13	1	-2.628157	2.244483	0.000242
14	6	-5.204630	0.002375	0.000089
15	1	-4.981870	-2.131258	-0.000250
16	1	-5.113145	2.156957	0.000394
17	6	1.327570	0.425898	-0.000103
18	6	2.090564	0.351839	1.214009
19	6	2.090796	0.352268	-1.214096
20	6	3.439650	0.107476	1.225323
21	1	1.562453	0.461998	2.157493
22	6	3.439881	0.107910	-1.225237
23	1	1.562867	0.462757	-2.157643
24	6	4.163791	-0.032862	0.000088
25	1	3.957355	0.035282	2.173067
26	1	3.957767	0.036033	-2.172906
27	7	5.499143	-0.286078	0.000171
28	6	6.234474	-0.400375	-1.258057
29	1	6.199865	0.533284	-1.831177
30	1	7.277159	-0.627855	-1.041165
31	1	5.833020	-1.206755	-1.881456
32	6	6.234189	-0.401003	1.258508
33	1	5.832407	-1.207514	1.881522
34	1	7.276861	-0.628666	1.041748
35	1	6.199690	0.532453	1.831970
36	6	-6.674212	-0.039933	0.000214
37	8	-7.350610	-1.055489	0.000256
38	1	-7.161122	0.962619	0.000199

Energy = -955.4307349
E+ZPVE = -955.132606
Imaginary frequency: - 301.3

k: Diphenylimidoylketene 1 with substituents – NMe_2 on migrating –CN on non-migrating phenyl groups

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Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.506233	-1.119532	1.003631
2	8	-0.127389	-2.064295	1.571901
3	7	-0.469239	2.217965	-0.190167
4	1	0.312025	2.819635	-0.461813
5	6	-1.006556	-0.052154	0.368195
6	6	-0.039903	1.024946	0.022243
7	6	-2.480576	-0.041873	0.158861
8	6	-3.199125	1.157942	0.006562
9	6	-3.191664	-1.258454	0.114125
10	6	-4.576357	1.135178	-0.183617
11	1	-2.657743	2.094150	0.027185
12	6	-4.567497	-1.283704	-0.058017
13	1	-2.660899	-2.202439	0.203313
14	6	-5.277231	-0.080755	-0.212182
15	1	-5.119038	2.067042	-0.303494
16	1	-5.097380	-2.229673	-0.088841
17	6	1.401607	0.640439	-0.027109
18	6	1.854332	-0.512497	-0.689239
19	6	2.372420	1.475818	0.550206
20	6	3.204885	-0.823620	-0.769643
21	1	1.140127	-1.164466	-1.183550
22	6	3.724128	1.174046	0.490842
23	1	2.055295	2.370313	1.079409
24	6	4.182065	0.006377	-0.169473
25	1	3.500444	-1.712775	-1.311653
26	1	4.428153	1.843097	0.969152
27	7	5.523677	-0.308924	-0.221143
28	6	5.967682	-1.480947	-0.957154
29	1	5.742728	-1.412231	-2.031270
30	1	7.046882	-1.587001	-0.844445
31	1	5.500868	-2.395433	-0.571205
32	6	6.510034	0.617556	0.309536
33	1	6.361945	0.792974	1.382521
34	1	7.505988	0.194252	0.177748
35	1	6.484255	1.591094	-0.200225
36	6	-6.697045	-0.098340	-0.401061

37	7	-7.850772	-0.114287	-0.554156

Energy = -934.3933583
E+ZPVE = -934.103255

k: oxoketenimine 2 with –NMe_2 on migrating and –CN on non-migrating phenyl group

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Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.046525	-0.722051	-0.548174
2	8	-0.437361	-1.844478	-0.855028
3	7	-0.266829	2.732300	-1.188761
4	1	0.080162	3.433118	-0.531767
5	6	-1.034039	0.413361	-0.466063
6	6	-0.602431	1.640429	-0.759455
7	6	1.390201	-0.460396	-0.283166
8	6	2.338839	-1.329525	-0.851146
9	6	1.864754	0.554854	0.562492
10	6	3.694423	-1.168915	-0.630531
11	1	1.981790	-2.138108	-1.480270
12	6	3.219797	0.720868	0.809616
13	1	1.161752	1.201980	1.077633
14	6	4.179137	-0.127661	0.203725
15	1	4.385363	-1.855172	-1.103644
16	1	3.532966	1.501592	1.491109
17	6	-2.478757	0.190881	-0.201871
18	6	-2.939228	-1.005198	0.378661
19	6	-3.423638	1.192046	-0.499287
20	6	-4.287994	-1.186652	0.658523
21	1	-2.239439	-1.801284	0.592260
22	6	-4.771227	1.018279	-0.220333
23	1	-3.099086	2.118444	-0.963272
24	6	-5.219303	-0.177551	0.365805
25	1	-4.627375	-2.114170	1.107264
26	1	-5.484129	1.800243	-0.459160
27	7	5.528121	0.044646	0.420531
28	6	5.994843	1.078584	1.329591
29	1	5.656511	0.912136	2.362314
30	1	7.084932	1.090757	1.329127
31	1	5.650167	2.071280	1.015489
32	6	6.482348	-0.909181	-0.123562
33	1	6.432304	-0.947668	-1.218653
34	1	7.491455	-0.602615	0.152274
35	1	6.318120	-1.925390	0.260465
36	6	-6.609124	-0.363621	0.657919
37	7	-7.738300	-0.511321	0.898602

Energy = - 934.3921754
E+ZPVE = -934.103098

k: TS1 with –NMe_2 on migrating and –CN on non-migrating phenyl group

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Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.142851	1.223701	-0.000029
2	8	0.237471	2.440303	-0.000055
3	7	-0.134658	-2.140589	0.000041
4	1	-1.068908	-2.532236	0.000053
5	6	1.016140	0.108631	-0.000006
6	6	0.026143	-0.902299	0.000016
7	6	2.462316	0.001925	-0.000004
8	6	3.114430	-1.249019	0.000023
9	6	3.250061	1.174476	-0.000028
10	6	4.499560	-1.326546	0.000025
11	1	2.520327	-2.156924	0.000041
12	6	4.634286	1.097606	-0.000026
13	1	2.752915	2.138516	-0.000048
14	6	5.277283	-0.154411	0.000001
15	1	4.992403	-2.293393	0.000045
16	1	5.231186	2.003912	-0.000044
17	6	-1.243018	0.415591	-0.000010
18	6	-2.007289	0.356517	-1.214302
19	6	-2.007283	0.356568	1.214289
20	6	-3.360247	0.135550	-1.225472
21	1	-1.477490	0.458520	-2.157739
22	6	-3.360242	0.135602	1.225475
23	1	-1.477480	0.458611	2.157720
24	6	-4.086620	0.007353	0.000006
25	1	-3.879452	0.073325	-2.173084
26	1	-3.879441	0.073419	2.173093
27	7	-5.425745	-0.222703	0.000012
28	6	-6.163476	-0.321657	1.258368
29	1	-6.114890	0.613218	1.828459
30	1	-7.209309	-0.534168	1.041603
31	1	-5.774470	-1.132109	1.884235
32	6	-6.163477	-0.321688	-1.258342
33	1	-5.774495	-1.132179	-1.884174
34	1	-7.209317	-0.534156	-1.041569
35	1	-6.114860	0.613161	-1.828472
36	6	6.706010	-0.235158	0.000003
37	7	7.868823	-0.301905	0.000005

Energy = -934.3487422
E+ZPVE = -934.061301
Imaginary frequency: -298.6062

m: Diphenylimidoylketene 1 with substituents – NMe_2 on migrating –NO_2 on non-migrating phenyl groups

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.077716	-1.123804	1.015139
2	8	0.307753	-2.076429	1.564221
3	7	-0.043376	2.234126	-0.116277
4	1	0.737580	2.838158	-0.383399
5	6	-0.585256	-0.045144	0.403143
6	6	0.382709	1.035644	0.068145
7	6	-2.059203	-0.031234	0.206393
8	6	-2.771187	1.170767	0.030783
9	6	-2.777048	-1.246836	0.193848
10	6	-4.150089	1.153361	-0.150825
11	1	-2.224008	2.103702	0.031351
12	6	-4.153595	-1.270066	0.029390
13	1	-2.251175	-2.191394	0.301858
14	6	-4.829197	-0.062505	-0.144667
15	1	-4.707544	2.071407	-0.288449
16	1	-4.708836	-2.199274	0.019142
17	6	1.821589	0.645457	-0.002690
18	6	2.262528	-0.495682	-0.692868
19	6	2.801789	1.464896	0.581801
20	6	3.610740	-0.810768	-0.793140
21	1	1.540753	-1.134240	-1.193716
22	6	4.151343	1.158656	0.502666
23	1	2.493949	2.349768	1.132238
24	6	4.597598	0.002771	-0.186058
25	1	3.896808	-1.689700	-1.356420
26	1	4.863089	1.814774	0.987345
27	7	5.936981	-0.316624	-0.257870
28	6	6.368822	-1.475611	-1.021489
29	1	6.133063	-1.384691	-2.091590
30	1	7.448686	-1.587810	-0.922140
31	1	5.902491	-2.395829	-0.648849
32	6	6.932628	0.594487	0.282381
33	1	6.795651	0.748144	1.360151
34	1	7.925333	0.169773	0.132142
35	1	6.906192	1.578379	-0.206946
36	8	-6.851814	-1.171189	-0.317436
37	8	-6.854371	1.003004	-0.482672
38	7	-6.282648	-0.077588	-0.328330

Energy = -1046.6521571
E+ZPVE = -1046.357982

Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1046.9869533
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1046.6927783

m: oxoketenimine 2 with $-NMe_2$ on migrating and $-NO_2$ on non-migrating phenyl group

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Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.372144	-0.674058	-0.633052
2	8	-0.020015	-1.774926	-1.008006
3	7	0.185224	2.804051	-1.116863
4	1	0.531320	3.474472	-0.428763
5	6	-0.611002	0.462723	-0.507184
6	6	-0.167029	1.698758	-0.740837
7	6	1.804511	-0.435771	-0.329012
8	6	2.758411	-1.282500	-0.921801
9	6	2.269320	0.533323	0.574525
10	6	4.110397	-1.142319	-0.668689
11	1	2.408374	-2.056540	-1.596634
12	6	3.620355	0.677538	0.854395
13	1	1.560911	1.158932	1.108528
14	6	4.585828	-0.146787	0.224819
15	1	4.805673	-1.809381	-1.162428
16	1	3.925514	1.421422	1.579443
17	6	-2.058506	0.240304	-0.266874
18	6	-2.536823	-0.990257	0.223323
19	6	-2.988452	1.275176	-0.496513
20	6	-3.889646	-1.175123	0.482644
21	1	-1.848039	-1.808211	0.381528
22	6	-4.340362	1.101252	-0.239629
23	1	-2.648368	2.228085	-0.889849
24	6	-4.778806	-0.127874	0.251672
25	1	-4.265313	-2.117303	0.861246
26	1	-5.058383	1.891756	-0.417085
27	7	5.931209	0.005363	0.474324
28	6	6.386732	0.988346	1.443745
29	1	6.027273	0.771596	2.459788
30	1	7.476647	0.992727	1.464680
31	1	6.054204	1.998067	1.174066
32	6	6.890345	-0.925509	-0.100399
33	1	6.857926	-0.909903	-1.196651
34	1	7.895984	-0.637515	0.206299

35	1	6.715900	-1.958470	0.230706
36	8	-6.564512	-1.418620	0.955745
37	8	-6.963759	0.627976	0.317720
38	7	-6.204696	-0.320630	0.527490

Energy = -1046.6509171
E+ZPVE = -1046.357761

Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1046.986117
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1046.692961

m: TS1 with $-NMe_2$ on migrating and $-NO_2$ on non-migrating phenyl group

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.282808	1.242496	0.000333
2	8	-0.189985	2.458804	0.000727
3	7	-0.547819	-2.124020	-0.000919
4	1	-1.480288	-2.520133	-0.000781
5	6	0.595516	0.129353	-0.000067
6	6	-0.391523	-0.885932	-0.000398
7	6	2.039695	0.027825	-0.000060
8	6	2.695661	-1.223217	-0.000295
9	6	2.822895	1.205630	0.000205
10	6	4.080552	-1.297552	-0.000240
11	1	2.104089	-2.132545	-0.000519
12	6	4.207122	1.135484	0.000231
13	1	2.321443	2.167239	0.000404
14	6	4.827045	-0.117019	0.000015
15	1	4.597307	-2.249055	-0.000381
16	1	4.819322	2.028595	0.000426
17	6	-1.663957	0.430984	0.000109
18	6	-2.427786	0.367420	-1.214555
19	6	-2.427671	0.366431	1.214793
20	6	-3.778547	0.134798	-1.225618
21	1	-1.899064	0.474981	-2.157960
22	6	-3.778427	0.133753	1.225796
23	1	-1.898862	0.473247	2.158234
24	6	-4.503870	-0.000255	0.000069
25	1	-4.297270	0.068968	-2.173207
26	1	-4.297063	0.067158	2.173381
27	7	-5.840519	-0.241468	0.000002
28	6	-6.577502	-0.348407	1.258433
29	1	-6.536662	0.586127	1.829561
30	1	-7.621483	-0.569270	1.041296
31	1	-6.181672	-1.156497	1.882989
32	6	-6.577568	-0.346893	-1.258531

33	1	-6.182091	-1.154541	-1.883890
34	1	-7.621644	-0.567474	-1.041598
35	1	-6.536289	0.588186	-1.828721
36	8	6.805746	-1.313119	0.000274
37	8	6.920354	0.864354	-0.000293
38	7	6.283818	-0.193751	0.000027

Energy = -1046.6083556
E+ZPVE = -1046.316830
Imaginary frequency: -294.3

Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1046.9444129
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1046.6528869

n: diphenylimidoylketene1 with–NHMe on migrating and –SO2CN on non-migrating phenyl group:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.135163	-1.095057	0.993889
2	8	1.515612	-2.044412	1.550278
3	7	1.159103	2.266547	-0.125849
4	1	1.939662	2.882532	-0.364883
5	6	0.629262	-0.020949	0.370810
6	6	1.593876	1.073294	0.069596
7	6	-0.836797	-0.025609	0.130196
8	6	-1.545973	1.164880	-0.121188
9	6	-1.546835	-1.246195	0.142599
10	6	-2.918459	1.133725	-0.346779
11	1	-1.000794	2.099161	-0.142222
12	6	-2.917143	-1.285507	-0.065902
13	1	-1.020430	-2.183030	0.301554
14	1	-3.461270	2.049493	-0.554197
15	1	-3.454140	-2.227383	-0.067121
16	6	3.038806	0.700563	0.045723
17	6	3.514002	-0.429049	-0.638629
18	6	3.987096	1.532309	0.672183
19	6	4.871206	-0.726414	-0.700468
20	1	2.815297	-1.071285	-1.166793
21	6	5.338426	1.239652	0.632569
22	1	3.647508	2.407059	1.219754
23	6	5.814257	0.099653	-0.055919
24	1	5.198078	-1.596946	-1.256944
25	1	6.047002	1.884093	1.146933
26	7	7.160142	-0.184205	-0.059274
27	1	7.769352	0.560819	0.240346

28	6	7.756439	-1.218558	-0.879863
29	1	7.568176	-1.076291	-1.954321
30	1	8.835712	-1.216081	-0.717077
31	1	7.380691	-2.208216	-0.596297
32	8	-5.757650	1.075715	-1.314935
33	8	-5.747219	-1.467235	-1.011082
34	6	-5.990088	0.068770	1.062941
35	7	-6.431367	0.192910	2.131183
36	16	-5.345890	-0.125857	-0.594757
37	6	-3.595187	-0.087092	-0.309945

Energy = -1443.622768
E+ZPVE = -1443.351354
E+ Gcorrection = -1443.405838
Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1444.0347398
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1443.7633258
E+ Gcorrection (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1443.8178098

n: oxoketenimine 2 with –NHMe on migrating and –SO2CN on non-migrating phenyl group:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.547465	-0.778763	-0.540892
2	8	1.097444	-1.899427	-0.759526
3	7	1.519071	2.601671	-1.502342
4	1	1.912142	3.346933	-0.926050
5	6	0.621233	0.412011	-0.562505
6	6	1.120287	1.580216	-0.971401
7	6	2.992934	-0.570810	-0.284433
8	6	3.897460	-1.535771	-0.773046
9	6	3.510496	0.485219	0.481299
10	6	5.254085	-1.422945	-0.548367
11	1	3.501089	-2.371418	-1.339881
12	6	4.871977	0.601060	0.733811
13	1	2.836185	1.206859	0.931814
14	6	5.776780	-0.346062	0.208978
15	1	5.936378	-2.166282	-0.953528
16	1	5.232637	1.416018	1.350586
17	6	-0.830015	0.298501	-0.278685
18	6	-1.361777	-0.842073	0.354274
19	6	-1.705645	1.353904	-0.607843
20	6	-2.716911	-0.922081	0.653524
21	1	-0.712780	-1.671570	0.597043
22	6	-3.060117	1.286117	-0.315411
23	1	-1.321360	2.239630	-1.103747
24	6	-3.556652	0.141956	0.316130

25	1	-3.119431	-1.794750	1.155872
26	1	-3.725440	2.105857	-0.562276
27	7	7.131177	-0.245506	0.403373
28	1	7.680489	-1.050600	0.147222
29	6	7.751647	0.719109	1.287522
30	1	7.406631	0.627105	2.327584
31	1	8.832159	0.566469	1.270155
32	1	7.554802	1.744008	0.952146
33	16	-5.284616	0.048715	0.707852
34	8	-5.854940	1.393231	0.735323
35	8	-5.495728	-0.914754	1.784635
36	6	-5.956008	-0.721627	-0.759696
37	7	-6.418432	-1.218718	-1.703257

Energy = -1443.6215646
E+ZPVE = -1443.351312
E+ Gcorrection = -1443.40632
Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1444.033629
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1443.763377
E+ Gcorrection (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1443.81839

n: TS1 with–NHMe on migrating and –SO2CN on non-migrating phenyl group:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.500187	1.254974	0.055289
2	8	-1.421190	2.454012	0.262996
3	7	-1.712222	-2.064064	-0.540757
4	1	-2.636236	-2.476249	-0.595199
5	6	-0.606532	0.172442	-0.149185
6	6	-1.578091	-0.844168	-0.317874
7	6	0.837266	0.096049	-0.186493
8	6	1.506668	-1.126350	-0.418308
9	6	1.603117	1.269678	0.007670
10	6	2.892197	-1.180479	-0.449500
11	1	0.925169	-2.028179	-0.576985
12	6	2.988202	1.223350	-0.022958
13	1	1.087962	2.208903	0.176993
14	6	3.625431	-0.003975	-0.249939
15	1	3.409016	-2.115002	-0.638487
16	1	3.577854	2.123376	0.112996
17	6	-2.867326	0.432019	-0.068307
18	6	-3.650087	0.570340	-1.268972
19	6	-3.602001	0.132111	1.129269
20	6	-4.992039	0.307538	-1.295320
21	1	-3.139714	0.858180	-2.184017
22	6	-4.947944	-0.135851	1.121404

23	1	-3.052958	0.081547	2.065785
24	6	-5.678833	-0.060463	-0.099113
25	1	-5.555319	0.388490	-2.221595
26	1	-5.459109	-0.390119	2.042555
27	7	-7.003244	-0.322678	-0.149308
28	1	-7.456497	-0.229949	-1.045835
29	6	-7.834493	-0.681483	0.988263
30	1	-7.843129	0.110256	1.745785
31	1	-8.855851	-0.831938	0.637580
32	1	-7.491649	-1.611103	1.455832
33	16	5.390043	-0.070234	-0.288689
34	8	5.830455	-1.266854	-1.003080
35	8	5.936209	1.254447	-0.575686
36	6	5.794873	-0.379307	1.429272
37	7	6.078987	-0.581239	2.538436

Energy = -1443.5801865
E+ZPVE = -1443.311332
E+ Gcorrection = -1443.364556
Imaginary frequency: -285.0cm^{-1}
Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1443.9925265
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1443.7236725
E+ Gcorrection (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1443.7768955

a: oxoketene 3 H/H:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.128911	1.618703	-0.151135
2	8	0.166122	2.743262	-0.242066
3	6	-0.515202	0.343742	-0.065145
4	6	0.495817	-0.747758	-0.159863
5	6	-1.982580	0.074653	-0.004815
6	6	-2.473269	-1.024870	0.717115
7	6	-2.896779	0.926121	-0.645122
8	6	-3.844961	-1.258044	0.792203
9	1	-1.780282	-1.701130	1.201399
10	6	-4.268396	0.696697	-0.553266
11	1	-2.533648	1.768389	-1.228550
12	6	-4.748656	-0.398686	0.164524
13	1	-4.208335	-2.116730	1.349224
14	1	-4.959023	1.368334	-1.054651
15	1	-5.816457	-0.584707	0.229723
16	6	1.952093	-0.415333	-0.022563
17	6	2.432770	0.561939	0.860495

18	6	2.865040	-1.167084	-0.778382
19	6	3.803509	0.803285	0.962803
20	1	1.747169	1.108321	1.500319
21	6	4.229966	-0.914992	-0.684637
22	1	2.481669	-1.941517	-1.434067
23	6	4.701823	0.073157	0.184904
24	1	4.167702	1.553743	1.657760
25	1	4.928744	-1.490077	-1.284758
26	1	5.767910	0.265422	0.261991
27	8	0.142749	-1.900666	-0.370570

Energy = -728.0565719

E+ZPVE = -727.850564
Energy at (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -728.2854122
E+ZPVE (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -728.0794042

a: TS2 connecting oxoketene H/H and oxoketene H/H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.379195	-1.051560	-0.000012
2	8	0.465691	-2.246923	-0.000026
3	6	-0.556190	0.000149	-0.000001
4	6	0.378988	1.052002	0.000013
5	6	-2.016796	0.000008	-0.000002
6	6	-2.732241	1.211459	0.000011
7	6	-2.732018	-1.211573	-0.000015
8	6	-4.125042	1.205845	0.000010
9	1	-2.188897	2.151076	0.000022
10	6	-4.124820	-1.206209	-0.000016
11	1	-2.188505	-2.151091	-0.000025
12	6	-4.828708	-0.000247	-0.000004
13	1	-4.662965	2.149661	0.000020
14	1	-4.662571	-2.150124	-0.000027
15	1	-5.914625	-0.000347	-0.000005
16	6	1.789318	0.000245	0.000002
17	6	2.529805	0.000181	-1.218768
18	6	2.529803	0.000151	1.218772
19	6	3.915155	-0.000155	-1.218097
20	1	1.984432	0.000253	-2.158926
21	6	3.915153	-0.000185	1.218103
22	1	1.984430	0.000201	2.158929
23	6	4.607728	-0.000301	0.000003
24	1	4.464838	-0.000283	-2.154186
25	1	4.464835	-0.000335	2.154193
26	1	5.693926	-0.000498	0.000004

27	8	0.465449	2.247251	0.000028

Energy = -728.0101343
E+ZPVE = -727.805915
Imaginary Frequency: -389.2
Energy at (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -728.2374561
E+ZPVE (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -728.0332371

m: oxoketene 3 with $-NMe_2$ on migrating and $-NO_2$ on non-migrating phenyl group

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Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.144867	1.317219	1.083107
2	8	-0.219711	2.278653	1.631937
3	6	0.597786	0.208096	0.492304
4	6	-0.387101	-0.903921	0.254626
5	6	2.061380	0.114888	0.248687
6	6	2.726084	-1.125491	0.213215
7	6	2.812713	1.290890	0.045091
8	6	4.095451	-1.183386	-0.022585
9	1	2.157036	-2.031509	0.365873
10	6	4.182126	1.241638	-0.171953
11	1	2.316604	2.257423	0.042839
12	6	4.810443	-0.002244	-0.207225
13	1	4.618646	-2.130859	-0.054641
14	1	4.765603	2.139952	-0.328030
15	6	-1.820112	-0.561667	0.087887
16	6	-2.284579	0.656063	-0.436971
17	6	-2.778073	-1.539545	0.413183
18	6	-3.639136	0.907028	-0.595779
19	1	-1.580353	1.410190	-0.773799
20	6	-4.132419	-1.301523	0.273591
21	1	-2.429777	-2.495843	0.788897
22	6	-4.607130	-0.060733	-0.228921
23	1	-3.945927	1.852294	-1.024568
24	1	-4.830861	-2.079718	0.554013
25	8	-0.006538	-2.070251	0.225289
26	7	6.255815	-0.065145	-0.445950
27	8	6.858074	0.998809	-0.602224
28	8	6.785250	-1.176909	-0.476123
29	7	-5.953113	0.187394	-0.362465
30	6	-6.411333	1.454999	-0.909037
31	1	-6.081881	1.602378	-1.946842
32	1	-7.500968	1.478482	-0.894589

33	1	-6.049329	2.302379	-0.313832
34	6	-6.923671	-0.851247	-0.052376
35	1	-7.928358	-0.463137	-0.219813
36	1	-6.793394	-1.739507	-0.684930
37	1	-6.856321	-1.167075	0.996231

Energy = -1066.5362192
E+ZPVE = -1066.254446.

Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1066.8813563
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1066.5995833

m: TS2 with $-NMe_2$ on migrating and –CN on non-migrating phenyl group:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.336086	-1.052207	-0.000010
2	8	-0.387714	-2.257511	-0.000018
3	6	0.614112	-0.000016	-0.000006
4	6	-0.336096	1.052151	-0.000005
5	6	2.064000	0.000000	-0.000004
6	6	2.782062	1.215678	0.000027
7	6	2.782082	-1.215667	-0.000032
8	6	4.169220	1.218364	0.000031
9	1	2.235515	2.152667	0.000049
10	6	4.169240	-1.218329	-0.000030
11	1	2.235551	-2.152665	-0.000056
12	6	4.851380	0.000023	0.000002
13	1	4.734753	2.141665	0.000057
14	1	4.734789	-2.141620	-0.000054
15	6	-1.662632	-0.000090	-0.000006
16	6	-2.437653	-0.000076	1.215399
17	6	-2.437663	-0.000093	-1.215406
18	6	-3.805663	-0.000043	1.226313
19	1	-1.902113	-0.000076	2.161449
20	6	-3.805672	-0.000062	-1.226310
21	1	-1.902129	-0.000123	-2.161460
22	6	-4.543032	-0.000042	0.000005
23	1	-4.329133	0.000014	2.173521
24	1	-4.329149	-0.000062	-2.173513
25	7	-5.899258	-0.000009	0.000008
26	6	-6.644541	0.000223	-1.258783
27	1	-6.418339	-0.889582	-1.856480
28	1	-7.711176	0.000239	-1.039953

29	1	-6.418252	0.890189	-1.856210
30	6	-6.644540	-0.000003	1.258799
31	1	-6.418634	0.890097	1.856177
32	1	-7.711175	-0.000478	1.039969
33	1	-6.417955	-0.889674	1.856545
34	8	6.890932	1.090206	0.000047
35	8	6.890950	-1.090126	-0.000032
36	7	6.312865	0.000035	0.000006
37	8	-0.387779	2.257476	-0.000003

Energy = -1066.5046661
E+ZPVE = -1066.223761
Imaginary Frequency: -136.3410

Energy at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1066.8496396
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d,p) = -1066.5687346

n: oxoketene 3 with –NHMe on migrating and –SO2CN on non-migrating phenyl group:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.089050	-1.298920	1.014676
2	8	1.462917	-2.266771	1.543983
3	6	0.623040	-0.183137	0.445424
4	6	1.591375	0.955016	0.262955
5	6	-0.835672	-0.111905	0.175382
6	6	-1.512517	1.121134	0.113151
7	6	-1.567207	-1.299876	-0.033575
8	6	-2.878619	1.161536	-0.145991
9	1	-0.954930	2.034713	0.264059
10	6	-2.933281	-1.270773	-0.275165
11	1	-1.058549	-2.259694	-0.024156
12	1	-3.398438	2.111316	-0.208249
13	1	-3.489068	-2.185829	-0.446426
14	6	3.032985	0.644725	0.117384
15	6	3.528744	-0.545501	-0.439229
16	6	3.963606	1.633281	0.500040
17	6	4.892723	-0.767743	-0.579313
18	1	2.844029	-1.297905	-0.817467
19	6	5.320926	1.419953	0.381286
20	1	3.586883	2.568065	0.901103
21	6	5.820873	0.207713	-0.156345
22	1	5.238023	-1.689753	-1.032002
23	1	6.022106	2.185769	0.703683
24	7	7.173695	0.011593	-0.245708
25	1	7.758613	0.812411	-0.067576

26	6	7.788927	-1.127820	-0.894106
27	1	7.517996	-1.207436	-1.956510
28	1	8.873358	-1.027823	-0.823927
29	1	7.506699	-2.063687	-0.398005
30	8	-5.692290	1.337617	-1.164016
31	8	-5.740414	-1.219517	-1.304518
32	6	-6.003566	-0.059270	0.998895
33	7	-6.467364	-0.111809	2.063489
34	16	-5.324546	0.020133	-0.653949
35	6	-3.579474	-0.032498	-0.329054
36	8	1.188565	2.114140	0.262763

Energy = -1463.5066012
E+ZPVE = -1463.247688
E+ Gcorrection = -1463.302450
Energy at (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -1463.9283087
E+ZPVE (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -1463.6693957
E+ Gcorrection (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -1463.7241577

n: TS2 with –NHMe on migrating and –SO2CN on non-migrating phenyl group:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.541448	1.053081	-0.166311
2	8	-1.590575	2.258196	-0.170015
3	6	-0.591402	0.000195	-0.178234
4	6	-1.541473	-1.052658	-0.167053
5	6	0.857115	0.000150	-0.200148
6	6	1.572689	-1.217133	-0.214108
7	6	1.572756	1.217406	-0.213191
8	6	2.959886	-1.221539	-0.234556
9	1	1.024573	-2.153163	-0.213014
10	6	2.959954	1.221750	-0.233628
11	1	1.024685	2.153461	-0.211392
12	6	3.644012	0.000090	-0.241712
13	1	3.513725	-2.153629	-0.258128
14	1	3.513847	2.153826	-0.256484
15	6	-2.864975	0.000336	-0.145031
16	6	-3.660199	0.000725	-1.351960
17	6	-3.614054	-0.000114	1.087333
18	6	-5.025118	0.000507	-1.331157
19	1	-3.140161	0.001161	-2.306367
20	6	-4.982956	-0.000339	1.127241
21	1	-3.056771	-0.000325	2.020717
22	6	-5.727711	-0.000053	-0.087922
23	1	-5.594708	0.000767	-2.257021
24	1	-5.501551	-0.000720	2.078714

25	7	-7.076658	-0.000288	-0.090736
26	1	-7.534219	-0.000019	-0.990080
27	6	-7.923254	-0.000832	1.091858
28	1	-7.751650	0.889610	1.706476
29	1	-8.965444	-0.000953	0.771674
30	1	-7.751275	-0.891588	1.705914
31	16	5.413382	0.000044	-0.270306
32	8	5.903520	-1.279805	-0.776511
33	8	5.903609	1.280341	-0.775291
34	6	5.814756	-0.000805	1.474970
35	7	6.097642	-0.001366	2.602587
36	8	-1.590744	-2.257750	-0.171609

Energy = -1463.4759465
E+ZPVE = --1463.217735
E+ Gcorrection = -1463.270224
Imaginary Frequency: -124.2 cm^{-1}
Energy at (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -1463.8972069
E+ZPVE (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -1463.6389959
E+ Gcorrection (B3LYP/6-311+G (3df,2p)// B3LYP/6-31G (d,p) = -1463.6914839

Phenyloxoketene (B3LYP/6-31G*)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.431944	-0.833309	0.236211
2	8	-2.595686	-1.935677	0.579201
3	6	-2.271214	0.424648	-0.151973
4	6	-0.992116	1.171563	-0.193903
5	6	0.309081	0.430290	-0.118883
6	6	0.474880	-0.880006	-0.588736
7	6	1.412734	1.112893	0.415376
8	6	1.719020	-1.506105	-0.501843
9	1	-0.349985	-1.404673	-1.061489
10	6	2.649759	0.482948	0.512127
11	1	1.275268	2.135437	0.751378
12	6	2.804671	-0.829519	0.055532
13	1	1.840800	-2.517838	-0.878374
14	1	3.495708	1.013922	0.939885
15	1	3.771807	-1.319909	0.126599
16	8	-1.017701	2.392484	-0.270737
17	1	-3.175730	0.998183	-0.329157

Energy = -496.9877982
E+ZPVE = -496.862946
E at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d) = - 497.1623946

E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d) = -497.1043654

TS connecting phenyl oxoketene H/H and phenyloxoketene H/H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.495562	1.059475	-0.000014
2	8	1.402649	2.250808	-0.000028
3	6	2.407495	0.000000	-0.000002
4	6	1.495562	-1.059475	0.000012
5	6	0.062506	0.000000	0.000000
6	6	-0.675267	-0.000015	-1.217626
7	6	-0.675266	0.000015	1.217627
8	6	-2.061784	-0.000015	-1.217597
9	1	-0.130595	-0.000026	-2.158985
10	6	-2.061783	0.000015	1.217600
11	1	-0.130592	0.000026	2.158986
12	6	-2.755136	0.000000	0.000002
13	1	-2.611239	-0.000026	-2.154683
14	1	-2.611236	0.000026	2.154687
15	1	-3.841912	0.000000	0.000003
16	8	1.402650	-2.250808	0.000026
17	1	3.491844	0.000000	-0.000003

Energy = -496.9307332
E+ZPVE = -496.807646
Imaginary Frequency: -434.6
E at (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d) = - 497.1043654
E+ZPVE (B3LYP/6-311+G(3df,2p)// B3LYP/6-31G(d) = -496.9812784